

Algorithms for estimating spectral density functions for periodic potentials on the half line

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Abstract

For Hill's equation on $[0, \infty)$ we prove new characterizations of the spectral function $\rho(\lambda)$ and the spectral density function $f(\lambda)$ based on analysis involving a companion system of first order differential equations as in [6, 7]. A numerical algorithm is derived and implemented based on coefficient approximation. Results for several examples, including the Mathieu equation, are presented.

1 Introduction

In this paper we consider Hill's equation, henceforth referred to as the *SL-equation*,

$$-y'' + q(x)y = \lambda y, \quad 0 \leq x < \infty, \quad (1.1)$$

where $q(x)$ is real valued and periodic with period ℓ , and we impose a boundary condition

$$y(0) \cos \alpha + y'(0) \sin \alpha = 0 \quad (1.2)$$

for some $\alpha \in [0, \pi)$.

Let a fundamental system of solutions for (1.1) be defined for all $\lambda \in \mathbb{C}$ by

$$\begin{bmatrix} \theta(0, \lambda) & \phi(0, \lambda) \\ \theta'(0, \lambda) & \phi'(0, \lambda) \end{bmatrix} = \begin{bmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{bmatrix}; \quad (1.3)$$

we can define a unique Titchmarsh-Weyl m -function by ($\operatorname{Im} \lambda \neq 0$)

$$\theta(x, \lambda) + m(\lambda)\phi(x, \lambda) \in L_2(0, \infty). \quad (1.4)$$

The *spectral function* is then defined for $\lambda \in [\Lambda, \infty)$ by the Titchmarsh-Kodaira formula

$$\rho(\lambda) = \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \int_{\Lambda}^{\lambda} \operatorname{Im} m(\mu + i\epsilon) d\mu, \quad (1.5)$$

where Λ is the cutoff point for which equation (1.1) is nonoscillatory in $(-\infty, \Lambda)$ and oscillatory in (Λ, ∞) , or equivalently, the lowest point of the essential spectrum. The *spectral density function* is then defined for $\lambda \in [\Lambda, \infty)$ by

$$f(\lambda) := \rho'(\lambda) = \frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \operatorname{Im}[m(\lambda + i\epsilon)]. \quad (1.6)$$

We now summarize some well known information on the spectrum associated with the problem (1.1)-(1.2) (see, for example, [5, Chap 1-2]). For the case of periodic potentials with the above boundary condition, the spectrum is known to be absolutely continuous and consisting of bands interspersed with open intervals called gaps. For the regular periodic problem having the boundary conditions

$$y(0) = y(\ell), \quad y'(0) = y'(\ell), \quad (1.7)$$

let the eigenvalues be ordered by $\lambda_0 \leq \lambda_1 \leq \dots$, where eigenvalues of multiplicity two are written twice in the sequence. For the regular semi-periodic problem having the boundary conditions

$$y(0) = -y(\ell), \quad y'(0) = -y'(\ell), \quad (1.8)$$

let the eigenvalues be ordered by $\mu_0 \leq \mu_1 \leq \dots$, where eigenvalues of multiplicity two are written twice in the sequence. Then the eigenvalues of the periodic and semi-periodic problems occur in the order

$$-\infty < \Lambda = \lambda_0 < \mu_0 \leq \mu_1 < \lambda_1 \leq \lambda_2 < \mu_2 \leq \mu_3 < \lambda_3 \leq \lambda_4 \dots$$

If A denotes the self-adjoint operator associated with the SL problem (1.1)-(1.2) then the closed intervals

$$[\lambda_0, \mu_0], [\mu_1, \lambda_1], [\lambda_2, \mu_2], [\mu_3, \lambda_3], \dots \quad (1.9)$$

constitute the essential spectrum σ_e (or the stability set) of A . The complementary set of open intervals

$$(\mu_0, \mu_1), (\lambda_1, \lambda_2), (\mu_2, \mu_3), \dots \quad (1.10)$$

are the gaps in σ_e , or the instability set. The spectral function $\rho(\lambda)$ in (1.5) is absolutely continuous and monotone increasing on σ_e , so the absolutely continuous spectrum is $\sigma_{ac}(A) = \sigma_e$.

In this paper we develop new characterizations for the spectral density function $f(\lambda)$; one leads to a very efficient algorithm for its calculation. In Section 2 we summarize some general information concerning the SL equation (1.1) and a companion system of first order equations which we will utilize in this paper. In Section 3 the new characterizations are derived. The remaining sections develop the numerical scheme and show examples.

2 Preliminaries

In this section we give the first order system of equations which we have found to be a useful companion system for the study of the Sturm-Liouville equation (the PQR-equations in [6],[7]), introduce a standard basis for the solution space, and state some relations which connect it to equation (1.1).

Consider the companion first order system for $U = (P, Q, R)^T$ for $\lambda \in (\Lambda, \infty)$:

$$\frac{dU}{dx} = \frac{d}{dx} \begin{bmatrix} P \\ Q \\ R \end{bmatrix} = \begin{bmatrix} 0 & \lambda - q & 0 \\ -2 & 0 & 2(\lambda - q) \\ 0 & -1 & 0 \end{bmatrix} \cdot \begin{bmatrix} P \\ Q \\ R \end{bmatrix}. \quad (2.1)$$

The following statements are straightforward, if occasionally tedious, to verify.

1. If y is any solution of the SL-equation, then $((y')^2, -2yy, y^2)$ is a solution of equation (2.1).
2. If we let a fundamental system of the SL-equation be defined by the initial conditions,

$$\begin{bmatrix} u(0, \lambda) & v(0, \lambda) \\ u'(0, \lambda) & v'(0, \lambda) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad (2.2)$$

then a corresponding fundamental system of solutions of equation (2.1) is

$$U = [U_1, U_2, U_3] = \begin{bmatrix} (u')^2 & u'v' & (v')^2 \\ -2uu' & -[u'v + uv'] & -2vv' \\ u^2 & uv & v^2 \end{bmatrix}. \quad (2.3)$$

3. If we represent a general solution of equation (2.1) in the form

$$\begin{bmatrix} P \\ Q \\ R \end{bmatrix} = a(\lambda)U_1(x, \lambda) + b(\lambda)U_2(x, \lambda) + c(\lambda)U_3(x, \lambda), \quad (2.4)$$

then (using the initial conditions (2.2)) we have

$$a(\lambda) = R(0, \lambda), \quad b(\lambda) = -Q(0, \lambda), \quad c(\lambda) = P(0, \lambda). \quad (2.5)$$

4. The solutions $\{\theta, \phi\}$ defined by the initial conditions (1.3) are linearly related to the solutions $\{u, v\}$ (and vice versa) by

$$\theta = u \cos \alpha + v \sin \alpha, \quad \phi = -u \sin \alpha + v \cos \alpha, \quad (2.6)$$

$$u = \theta \cos \alpha - \phi \sin \alpha, \quad v = \theta \sin \alpha + \phi \cos \alpha. \quad (2.7)$$

5. An indefinite inner product on the solution space of equation (2.1) may be defined by

$$\langle U_1, U_2 \rangle := 2(P_1R_2 + P_2R_1) - Q_1Q_2 = \text{const}, \text{ independent of } x \in [0, \infty) \quad (2.8)$$

where $U_k = (P_k, Q_k, R_k), k = 1, 2$.

6. For any solution $U = (P, Q, R)^T$ of equation (2.1),

$$\frac{d}{dx} \langle U, U \rangle = \frac{d}{dx} [4PR - Q^2] = 0,$$

i.e.

$$4PR - Q^2 = \text{const}, \text{ independent of } x \in [0, \infty) \quad (2.9)$$

7. If U_1 and U_2 are any two solutions of equation (2.1) represented as in (2.4), then

$$\langle U_1, U_2 \rangle = 2(a_1c_2 + c_1a_2) - b_1b_2 \quad (2.10)$$

and, in particular,

$$\langle U_1, U_1 \rangle = 4a_1c_1 - b_1^2. \quad (2.11)$$

8. If $U = (P, Q, R)^T$ is any solution of equation (2.1) expressed as in (2.4), then

$$\langle U, U \rangle = 4PR - Q^2 = 4ac - b^2. \quad (2.12)$$

9. If $U = (P, Q, R)^T$ is any solution of equation (2.1) expressed as in (2.4), and if it is also written as

$$U = \gamma_1 V_1 + \gamma_2 V_2 + \gamma_3 V_3$$

where

$$V = [V_1, V_2, V_3] = \begin{bmatrix} (\theta')^2 & \theta'\phi' & (\phi')^2 \\ -2\theta\theta' & -[\theta'\phi + \theta\phi'] & -2\phi\phi' \\ \theta^2 & \theta\phi & \phi^2 \end{bmatrix} \quad (2.13)$$

is the fundamental system of (2.1) generated by the solutions $\{\theta, \phi\}$ defined by (1.3), then

$$4ac - b^2 = 4\gamma_1\gamma_3 - \gamma_2^2. \quad (2.14)$$

In fact, the result holds if θ and ϕ are any two solutions of the SL-equation with $W_x(\theta(\cdot, \lambda), \phi(\cdot, \lambda)) = 1$.

10. If y is any solution of the SL equation (1.1) and $U = (P, Q, R)^T$ is any solution of companion system (2.1) then

$$\frac{d}{dx}[Py^2 + Qyy' + R(y')^2] = 0,$$

i.e.,

$$P(x, \lambda)y^2(x, \lambda) + Q(x, \lambda)y(x, \lambda)y'(x, \lambda) + R(x, \lambda)(y'(x, \lambda))^2 = \text{constant, independent of } x. \quad (2.15)$$

In the proofs in the next sections we will make frequent use of the above results (particularly **1**) which relate the solutions of the SL-equation to the solutions of the companion system (2.1). We exploited similar interrelations in [6] and [7] in the study of potentials on the half line satisfying $q \in L_1(0, \infty)$. Here we make use of the same interrelations in the study of periodic potentials.

Remark : In our previous papers [6], [7] the system (2.1) was referred to as the “PQR equations” (our notation); however, the analysis leading to them (particularly the motivating property (2.15)) was discovered by M. Appell [3] in 1880. Accordingly, we will henceforth refer to this first order system as the Appell equations.

3 Characterizations of the spectral density function

In this section we give an analog of the closed form characterization obtained in [7] when $q \in L_1(0, \infty)$. For the case of a periodic potential on the half line $[0, \infty)$ the basic ideas from [1], [2], [6], and [7] carry over, at least for values of λ in the stability intervals, to yield several formulas for the spectral density function.

We begin with the following definition as in [1].

DEFINITION. The Sturm-Liouville equation (1.1), with $q(x)$ periodic of period ℓ , satisfies *Condition A* for a given real value of λ if and only if there exists a complex-valued solution $y(x, \lambda)$ for which

$$\lim_{N \rightarrow \infty} \frac{\int_0^N y(x, \lambda)^2 dx}{\int_0^N |y(x, \lambda)|^2 dx} = 0. \quad (3.1)$$

We now have the following lemmas.

LEMMA 1. For λ in the stability intervals, let

$$\psi_1(x, \lambda) = p_1(x) \exp(ik(\lambda)x) \quad (3.2)$$

be the first Floquet solution for the characteristic exponent $\rho_1 = \exp(i\ell k(\lambda))$. Here the first Floquet solution for each λ is understood to have the choice of $k(\lambda)$ such that $0 < \ell k(\lambda) < \pi$, and $p_1(x)$ is periodic of period ℓ . Then

$$\lim_{N \rightarrow \infty} \frac{\int_0^N \psi_1(x, \lambda)^2 dx}{\int_0^N |\psi_1(x, \lambda)|^2 dx} = 0 \quad (3.3)$$

It follows from [1, Theorem 2] that the spectrum of (1.1) with (1.2) is absolutely continuous in the stability intervals.

PROOF.

$$\begin{aligned} \int_0^{m\ell} \psi_1^2 dx &= [1 + \sum_{j=1}^{m-1} \exp(2ij\ell k(\lambda))] \int_0^\ell \exp(2ik(\lambda)t) p_1^2(t) dt \\ &= \frac{1 - [\exp(2i\ell k(\lambda))]^m}{1 - \exp(2i\ell k(\lambda))} \int_0^\ell \exp(2ik(\lambda)t) p_1^2(t) dt. \end{aligned}$$

But $0 < k < \pi/\ell$, so $\exp(2i\ell k(\lambda)) \neq 1$ for λ in the stability intervals; hence, the ratio is bounded above. It follows that

$$\frac{\left| \int_0^{m\ell} \psi_1(x, \lambda)^2 dx \right|}{\int_0^{m\ell} |\psi_1(x, \lambda)|^2 dx} \leq \frac{K \int_0^\ell |p_1|^2 dt}{\int_0^{m\ell} |p_1|^2 dt} \rightarrow 0$$

as $m \rightarrow \infty$. \blacksquare

LEMMA 2. Let $\lambda \in \cup_{m=0}^\infty [\lambda_{2m}, \mu_{2m}] \cup [\mu_{2m+1}, \lambda_{2m+1}]$. Then, since Condition A holds for λ in these stability intervals, there is a complex-valued function $\xi(\lambda)$ that is uniquely defined for λ in the stability intervals by the properties

- (i) $\text{Im } \xi(\lambda) > 0$, and
- (ii)

$$\lim_{N \rightarrow \infty} \frac{\int_0^N (\theta(x, \lambda) + \xi(\lambda)\phi(x, \lambda))^2 dx}{\int_0^N |\theta(x, \lambda) + \xi(\lambda)\phi(x, \lambda)|^2 dx} = 0.$$

PROOF. This is proved in [1, Lemma1]. \blacksquare

Since the solution that satisfies Condition A is unique up to a constant multiple, it follows from Lemma 1 and Lemma 2 that there exists a constant $K \neq 0$ such that

$$\psi_1(x, \lambda) = K[\theta(x, \lambda) + \xi(\lambda)\phi(x, \lambda)]. \quad (3.4)$$

From (3.2) at $x = 0$ we have

$$\psi_1(0) \cos \alpha + \psi_1'(0) \sin \alpha = p_1(0) \cos \alpha + [ikp_1(0) + p_1'(0)] \sin \alpha.$$

But from (3.4)

$$\begin{aligned} \psi_1(0) \cos \alpha + \psi_1'(0) \sin \alpha &= K[\theta(0, \lambda) + \xi(\lambda)\phi(0, \lambda)] \cos \alpha + K[\theta'(0, \lambda) + \xi(\lambda)\phi'(0, \lambda)] \sin \alpha \\ &= K[\cos^2 \alpha - \xi \sin \alpha \cos \alpha + \sin^2 \alpha + \xi \sin \alpha \cos \alpha] \\ &= K. \end{aligned}$$

It also follows immediately from Theorem 2 of [1] that for all λ in the stability intervals, we have that the function $\xi(\lambda)$ is, in fact, the boundary value of the Titchmarsh-Weyl m -function defined in (1.4), that is,

$$\xi(\lambda) = A(\lambda) + iB(\lambda) := \lim_{\epsilon \rightarrow 0} m(\lambda + i\epsilon). \quad (3.5)$$

We are now ready to prove the following theorem:

THEOREM 1. For λ in the stability intervals, there exists a solution $U = (P, Q, R)^T$ of Appell's equation (2.1), unique up to a constant multiple, which is periodic of period ℓ on $(0, \infty)$.

PROOF. For λ in the stability intervals we set

$$U := \begin{bmatrix} P \\ Q \\ R \end{bmatrix} := \begin{bmatrix} \psi_1' \psi_2' \\ -(\psi_1 \psi_2' + \psi_2 \psi_1') \\ \psi_1 \psi_2 \end{bmatrix}, \quad (3.6)$$

where $\psi_1(x, \lambda) = p_1(x) \exp(ik(\lambda)x)$, and $\psi_2 = \overline{\psi_1}$. Since $p_1(x)$ is periodic of period ℓ , it follows that p_1' is also periodic of period ℓ . We obtain from (3.6) that

$$\begin{bmatrix} P \\ Q \\ R \end{bmatrix} = \begin{bmatrix} k(\lambda)^2 |p_1|^2 + |p_1'|^2 - 2k(\lambda) \operatorname{Im}(p_1 \overline{p_1'}) \\ -2\operatorname{Re}(p_1 \overline{p_1'}) \\ |p_1|^2 \end{bmatrix} \quad (3.7)$$

and each component is real valued and periodic with period ℓ .

To prove that the periodic solution is unique, up to constant multiple, consider the fundamental solution matrix of Appell's system of equations obtained by replacing $\{u, v\}$ in (2.3) by the Floquet solutions $\{\psi_1, \psi_2\}$, and let $T(x)$ be the transfer matrix which carries $U(x, \lambda)$ to $U(x + \ell, \lambda)$, i.e.

$$U(x + \ell, \lambda) = T(x)U(x, \lambda).$$

Since the Floquet solutions satisfy $\psi_j(x + \ell, \lambda) = \rho_j \psi_j(x, \lambda)$, where $\rho_j = \exp(\pm ik(\lambda)\ell)$, $j = 1, 2$, are the Floquet exponents for λ in the stability intervals, it follows that the first and third columns of (2.3) (with ψ_1 and ψ_2) are eigenvectors of $T(x)$ with eigenvalues ρ_1^2 and ρ_2^2 (which are not one), and the second column is an eigenvector of $T(x)$ with eigenvalue $\rho_1 \rho_2 = 1$. Hence T has a one-dimensional eigenspace for which P , Q and R are all periodic of period ℓ . ■

The next result provides three different representations for the spectral density function $f(\lambda)$.

THEOREM 2. For λ in a stability interval let $U = (P, Q, R)^T$ be the periodic solution of Appell's system (2.1) which is normalized by (compare (2.9))

$$\langle U, U \rangle = 4PR - Q^2 = 4. \quad (3.8)$$

Let $\{a(\lambda), b(\lambda), c(\lambda)\}$ be the coefficients in the representation (2.4) of this periodic solution. Then the spectral density function defined by (1.6) admits the following representations:

$$f(\lambda) = \left| \frac{1}{\pi[c(\lambda) \sin^2 \alpha + b(\lambda) \sin \alpha \cos \alpha + a(\lambda) \cos^2 \alpha]} \right| \quad (3.9)$$

$$= \left| \frac{1}{\pi[P(0, \lambda) \sin^2 \alpha - Q(0, \lambda) \sin \alpha \cos \alpha + R(0, \lambda) \cos^2 \alpha]} \right| \quad (3.10)$$

$$= \left| \frac{1}{\pi[P(x, \lambda)\phi(x, \lambda)^2 + Q(x, \lambda)\phi(x, \lambda)\phi'(x, \lambda) + R(x, \lambda)\phi'(x, \lambda)^2]} \right|. \quad (3.11)$$

Here it will be observed that the normalization (3.8) fixes the periodic solution only up to a \pm sign; it is for this reason that we take the absolute value sign in these formulas to ensure that $f(\lambda) \geq 0$, as required. In the applications it often happens that the denominators in the above expressions are positive in one stability interval and negative in another.

PROOF. The formulas (3.9) and (3.10) are equivalent because the representation (2.4) guarantees that $\{a(\lambda), b(\lambda), c(\lambda)\}$ are given by (2.5). The denominator in (3.11) is constant, independent of x , by (2.15) and equal to (3.10) on evaluation at $x = 0$. So it suffices to prove (3.10) subject to the normalization (3.8). Since $\psi_1(x, \lambda)$ is linearly dependent on $\theta(x, \lambda) + \xi(\lambda)\phi(x, \lambda)$ by (3.4) (where $\xi(\lambda)$ is the complex valued function defined on the stability intervals in Lemma 2), and $\psi_2 = \overline{\psi_1}$ is linearly dependent on $\theta(x, \lambda) + \overline{\xi(\lambda)}\phi(x, \lambda)$, we may represent the periodic solution in (3.6) as

$$U(x, \lambda) := \begin{bmatrix} P(x) \\ Q(x) \\ R(x) \end{bmatrix} := K(\lambda) \begin{bmatrix} (\theta' + \xi\phi')(\theta' + \overline{\xi}\phi') \\ -[(\theta + \xi\phi)(\theta' + \overline{\xi}\phi') + (\theta + \overline{\xi}\phi)(\theta' + \xi\phi')] \\ (\theta + \xi\phi)(\theta + \overline{\xi}\phi) \end{bmatrix} \quad (3.12)$$

for some real constant $K(\lambda)$, independent of x . The required normalization (3.8) is equivalent by (2.12) to

$$4a(\lambda)c(\lambda) - (b(\lambda))^2 = 4. \quad (3.13)$$

Using the representation of the periodic solution in terms of the fundamental system (2.13) of Appell's equations,

$$\begin{pmatrix} P \\ Q \\ R \end{pmatrix} = \gamma_1 V_1 + \gamma_2 V_2 + \gamma_3 V_3, \quad (3.14)$$

and comparing the R -component with the R -component in (3.12), gives

$$\gamma_1 = K(\lambda), \quad \gamma_2 = 2 \operatorname{Re}(\xi(\lambda))K(\lambda), \quad \text{and} \quad \gamma_3 = |\xi(\lambda)|^2 K(\lambda).$$

Hence from (2.12) and (2.14) we have

$$\begin{aligned} 4PR - Q^2 &= 4ac - b^2 \\ &= 4\gamma_1\gamma_3 - \gamma_2^2 \\ &= 4(K(\lambda))^2 \left[|\xi(\lambda)|^2 - \operatorname{Re}^2 \xi(\lambda) \right] \\ &= 4(K(\lambda))^2 \left[\operatorname{Im}^2 \xi(\lambda) \right] = 4 \end{aligned}$$

if and only if

$$[K(\lambda) \operatorname{Im} \xi(\lambda)]^2 = 1. \quad (3.15)$$

From (3.5) and (1.6) it follows (since $\operatorname{Im} \xi(\lambda) > 0$ by Lemma 2) that the normalization (3.8) holds if and only if

$$f(\lambda) := \frac{1}{\pi} \operatorname{Im} \xi(\lambda) = \frac{1}{\pi |K(\lambda)|}. \quad (3.16)$$

Next, we use the initial conditions (1.3) to evaluate the right hand side of (3.12) and then substitute into the denominator of (3.10) to obtain,

$$\begin{aligned} &\pi [P(0, \lambda) \sin^2 \alpha - Q(0, \lambda) \sin \alpha \cos \alpha + R(0, \lambda) \cos^2 \alpha] \\ &= \pi K(\lambda) \left[\frac{(\sin^2 \alpha + \cos^2 \alpha) \cdot 1}{+(\sin^3 \alpha \cos \alpha + \sin \alpha \cos^3 \alpha - \sin^3 \alpha \cos \alpha - \sin \alpha \cos^3 \alpha)(\xi + \bar{\xi})} \right. \\ &\quad \left. + (2 \sin^2 \alpha \cos^2 \alpha - 2 \sin^2 \alpha \cos^2 \alpha) |\xi|^2 \right] \\ &= \pi K(\lambda) \end{aligned} \quad (3.17)$$

The formula (3.10) now follows from (3.16) and (3.17). \blacksquare

A more useful characterization of $f(\lambda)$ is given by the following result.

THEOREM 3. Assume λ is in a stability interval. Then

$$f(\lambda) = \left| \frac{\sqrt{4 - [u(\ell, \lambda) + v'(\ell, \lambda)]^2}}{2\pi [u'(\ell, \lambda) \sin^2 \alpha + (u(\ell, \lambda) - v'(\ell, \lambda)) \cos \alpha \sin \alpha - v(\ell, \lambda) \cos^2 \alpha]} \right|. \quad (3.18)$$

Here the absolute value is needed to ensure that $f(\lambda) \geq 0$; this is due to the fact that the denominator could be negative in some of the stability intervals, and also corresponds to the fact that the normalization of $\{a, b, c\}$ in (3.19) fixes $\{a, b, c\}$ only up to a \pm sign.

PROOF. From Theorem 2 it follows that if we can construct a solution $U = (P, Q, R)^T$ of Appell's first order system (2.1) which is periodic of period ℓ and satisfies the normalization $4PR - Q^2 = 4$ then we can use it to get $f(\lambda)$ (e.g. from any one of the formulas (3.9), (3.10), or (3.11)). In particular, if this periodic solution is represented in the form (2.4) it follows from (2.12) that the coefficients $\{a, b, c\}$ satisfy

$$4a(\lambda)c(\lambda) - b^2(\lambda) = 4P(x, \lambda)R(x, \lambda) - Q(x, \lambda)^2 = 4. \quad (3.19)$$

Considering only the third component of (2.4) it therefore suffices to generate coefficients $\{a, b, c\}$ for which the quadratic form

$$R(x) = a(u(x, \lambda))^2 + bu(x, \lambda)v(x, \lambda) + c(v(x, \lambda))^2 \quad (3.20)$$

is periodic of period ℓ and such that (3.19) holds for λ in the stability intervals. Then $f(\lambda)$ is given by (3.9) with this choice of $\{a, b, c\}$; or by (3.10), (3.11) where $\{P, Q, R\}$ is the corresponding periodic solution (2.4) of Appell's equations. To manufacture $\{a, b, c\}$ consider the SL-equation (1.1) in the system form

$$\frac{d}{dx}\Psi = \begin{pmatrix} 0 & 1 \\ -(\lambda - q(x)) & 0 \end{pmatrix} \Psi = A(x) \cdot \Psi, \quad \Psi(x, \lambda) = \begin{pmatrix} y \\ y' \end{pmatrix}.$$

Let $\Psi_\alpha(\cdot, \lambda)$ be the solution of the initial value problem

$$\Psi'_\alpha(x) = A(x)\Psi_\alpha(x), \quad \Psi_\alpha(\alpha) = I, \quad \alpha \in [0, \infty). \quad (3.21)$$

The following facts are easily verified:

$$\Psi_0(x) = \begin{pmatrix} u(x) & v(x) \\ u'(x) & v'(x) \end{pmatrix} \quad (3.22)$$

$$[\Psi_0(x)]^{-1} = \Psi_x(0) \quad (3.23)$$

$$\forall \text{ solutions } y \text{ of (1.1)} : \begin{pmatrix} y(x) \\ y'(x) \end{pmatrix} = \Psi_0(x) \begin{pmatrix} y(0) \\ y'(0) \end{pmatrix} \quad (3.24)$$

$$\forall \text{ solutions } y \text{ of (1.1)} : \begin{pmatrix} y(0) \\ y'(0) \end{pmatrix} = \Psi_x(0) \begin{pmatrix} y(x) \\ y'(x) \end{pmatrix} \quad (3.25)$$

$$\Psi_\alpha(x) = \Psi_t(x) \cdot \Psi_\alpha(t) \quad (3.26)$$

The fact that $q(x)$ has period ℓ implies

$$\Psi_\ell(x + \ell) = \Psi_0(x), \quad (3.27)$$

and hence that $\Psi_x(x + \ell)$ is periodic with period ℓ . To generate a quadratic form in u and v which is periodic of period ℓ we put

$$\begin{aligned} \Phi(x) &:= \begin{pmatrix} 1 & 0 \end{pmatrix} \Psi_x(x + \ell) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \end{pmatrix} \Psi_\ell(x + \ell) \Psi_0(\ell) \Psi_x(0) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \end{pmatrix} \Psi_0(x) \Psi_0(\ell) \Psi_0(x)^{-1} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} u(x) & v(x) \end{pmatrix} \begin{bmatrix} u(\ell) & v(\ell) \\ u'(\ell) & v'(\ell) \end{bmatrix} \begin{pmatrix} -v(x) \\ u(x) \end{pmatrix} \end{aligned} \quad (3.28)$$

$$\begin{aligned} &= v(\ell)(u(x))^2 - [u(\ell) - v'(\ell)]u(x)v(x) - u'(\ell)(v(x))^2. \end{aligned} \quad (3.29)$$

$$= v(\ell)(u(x))^2 - [u(\ell) - v'(\ell)]u(x)v(x) - u'(\ell)(v(x))^2. \quad (3.30)$$

Since $\Phi(x + \ell) = \Phi(x)$ for all $x \in [0, \infty)$, we need only normalize the coefficients to achieve the required normalization (3.19). Taking $\gamma \cdot \Phi(x)$ so that $4ac - b^2 = 4$, we find

$$\gamma^2 [-4v(\ell)u'(\ell) - (u(\ell) - v'(\ell))^2] \quad (3.31)$$

$$= \gamma^2 [4 - (u(\ell) + v'(\ell))^2] \quad (3.32)$$

$$= 4, \quad (3.33)$$

so that the required normalization is achieved with

$$\begin{pmatrix} a(\lambda) \\ b(\lambda) \\ c(\lambda) \end{pmatrix} = \frac{1}{\sqrt{4 - (u(\ell) + v'(\ell))^2}} \begin{pmatrix} -2v(\ell) \\ 2(u(\ell) - v'(\ell)) \\ 2u'(\ell) \end{pmatrix}, \quad (3.34)$$

and substitution of this into (3.9) yields (3.18). ■

4 The Numerical Method

In this section and the following two sections we describe a new numerical algorithm for obtaining approximations to the spectral density function, by making use of the representation (3.18) in Theorem 3, and compare performance with **SLEDGE**. For general information and discussion of numerical methods for Sturm-Liouville problems we refer to Pryce's book [12], and for the computation of spectral functions using the method of **SLEDGE** we refer to our previous papers [10, 8, 4]. In contrast to **SLEDGE**, the above Theorem 3 for periodic potentials enables computation of the spectral density function on the stability intervals by shooting (with piecewise trigonometric / hyperbolic splines) over a single period.

To compute u and v we employ the method of coefficient approximation by which q is replaced by a step-function approximation \hat{q} . We write the analog to (1.1) as

$$-\hat{y}'' + \hat{q}(x)\hat{y} = \lambda\hat{y}, \quad a \leq x < \infty \quad (4.1)$$

and \hat{u} and \hat{v} will satisfy (4.1) with initial conditions analogous to those of u and v , respectively. We extend the formula (3.18) by defining for any λ

$$\hat{f}(\lambda) = \frac{\sqrt{\max\{0, 4 - [\hat{u}(\ell) + \hat{v}'(\ell)]^2\}}}{2\pi|\hat{u}'(\ell)\sin^2\alpha + (\hat{u}(\ell) - \hat{v}'(\ell))\sin\alpha\cos\alpha - \hat{v}(\ell)\cos^2\alpha|} \quad (4.2)$$

as an estimate of f . The appeal of this approach is that closed-form solutions, piecewise circular or hyperbolic trig functions, are known for \hat{u} and \hat{v} , admitting efficiencies of computation and analysis.

There are two potential numerical challenges in trying to integrate (4.1) and use (4.2): (1) mathematical instability when $\lambda < q(x)$, and (2) loss of accuracy if the numerator and denominator of (4.2) vanish simultaneously. We note that these difficulties arise in the original equations (1.1) and (3.18), so we would expect them to be inherited by any computational approach. With coefficient approximation it is straightforward to address both of these issues.

In [10] we presented a stabilizing algorithm to solve (4.1) for the regular Sturm-Liouville problem, which is a boundary value problem. A similar approach will work here. First, we provide more detail of the algorithm. We first subdivide $[0, \ell]$ into N intervals

$$0 = x_1 < x_2 < \cdots < x_{N+1} = \ell;$$

we set $h_n = x_{n+1} - x_n$ to be the width of the n th subinterval.

On any subinterval (x_n, x_{n+1}) we choose $\hat{q}(x) = q_n$ to be constant (usually the q value at the midpoint); then the differential equation (4.1) has the closed-form solution

$$\hat{y}(x) = \hat{y}(x_n)\phi'_n(x - x_n) + \hat{y}'(x_n)\phi_n(x - x_n) \quad (4.3)$$

with

$$\phi_n(t) = \begin{cases} \sin \omega_n t / \omega_n & \tau_n > 0 \\ \sinh \omega_n t / \omega_n & \tau_n < 0 \\ t & \tau_n = 0, \end{cases}$$

where

$$\tau_n = \lambda - q_n \quad (4.4)$$

and

$$\omega_n = \sqrt{|\tau_n|}.$$

It follows that

$$\hat{y}'(x) = -\tau_n \hat{y}(x_n) \phi_n(x - x_n) + \hat{y}'(x_n) \phi_n'(x - x_n). \quad (4.5)$$

In practice, one should use a truncated series expansion for small $|\tau_n| h_n^2$, e.g.,

$$\phi_n(t) = t[1 - \tau_n t^2/6 + \tau_n^2 t^4/120]$$

and only use the sin and sinh formulas when $|\tau_n| h_n^2$ is sufficiently large.

As a consequence, if we set

$$y_n := \hat{y}(x_n), \quad y_n' := \hat{y}'(x_n)$$

for any n , then we have the forward recurrence

$$\begin{bmatrix} y_{n+1} \\ y_{n+1}' \end{bmatrix} = \begin{bmatrix} \phi_n'(h_n) & \phi_n(h_n) \\ -\tau_n \phi_n(h_n) & \phi_n'(h_n) \end{bmatrix} \begin{bmatrix} y_n \\ y_n' \end{bmatrix}. \quad (4.6)$$

If we denote the coefficient matrix in (4.6) by A_n , it is not difficult to show that it has inverse

$$A_n^{-1} = \begin{bmatrix} \phi_n'(h_n) & -\phi_n(h_n) \\ \tau_n \phi_n(h_n) & \phi_n'(h_n) \end{bmatrix}. \quad (4.7)$$

Hence, a backward recurrence is

$$\begin{bmatrix} y_n \\ y_n' \end{bmatrix} = \begin{bmatrix} \phi_n'(h_n) & -\phi_n(h_n) \\ \tau_n \phi_n(h_n) & \phi_n'(h_n) \end{bmatrix} \begin{bmatrix} y_{n+1} \\ y_{n+1}' \end{bmatrix}. \quad (4.8)$$

It can be seen when $\tau_n > 0$ that A_n has eigenvalues $\cos(\omega_n h_n) \pm i \sin(\omega_n h_n)$ and spectral radius one. When $\tau_n < 0$, its eigenvalues are $\cosh(\omega_n h_n) \pm \sinh(\omega_n h_n)$ and its spectral radius is $\exp(\omega_n h_n)$. The exponential factor reflects the potential mathematical instability of the initial value problem (1.1) when $\lambda < q(x)$. To overcome this, define

$$\sigma_n = \begin{cases} \exp(\omega_n h_n) & \tau_n < -\epsilon \\ 1 & \text{otherwise,} \end{cases} \quad (4.9)$$

and for $j \leq k$

$$p(j, k) = \sigma_j \sigma_{j+1} \cdots \sigma_k. \quad (4.10)$$

Introduce the scaled variables

$$\tilde{y}_n = y_n / p(1, n-1) \quad (4.11)$$

$$\tilde{y}_n' = y_n' / p(1, n-1), \quad (4.12)$$

which satisfy the recurrences of the form (4.6) or (4.8) with coefficient matrix divided by σ_n . These scaled matrices have spectral radius one.

To use (4.6) requires an initial condition to start, while (4.8) requires a terminal condition. More generally, we define u^F and v^F to each satisfy the differential equation (4.1) with respective initial conditions $u^F(0) = 1$, $u^{F'}(0) = 0$ and $v^F(0) = 0$, $v^{F'}(0) = 1$. Similarly, u^B and v^B satisfy the same differential equation but with respective terminal conditions $u^B(\ell) = 1$, $u^{B'}(\ell) = 0$ and $v^B(\ell) = 0$, $v^{B'}(\ell) = 1$. We will define the 2-vector U^F to have components u^F and $u^{F'}$; furthermore, for $n =$

$1, 2, \dots, N+1$ let U_n^F denote the two-vector with components u_n^F and $u_n^{F'}$. Define 2-vectors $U^B, V^F, V^B, U_n^B, V_n^F$, and V_n^B analogously. For the vectors with B superscripts, we recur backwards from $n = N+1$ using (4.8) while for those with F superscripts we recur forwards from $n = 1$ using (4.6). Finally, we use a tilde overscore ($\tilde{}$) to denote the scaled versions of these recurrences. The analog of (4.11)–(4.12) for Y either U or V is

$$\tilde{Y}_n^F = Y_n^F / p(1, n-1) \quad (4.13)$$

$$\tilde{Y}_n^B = Y_n^B / p(n, N). \quad (4.14)$$

Since U^B and V^B form a basis of solutions for (4.1) there exist constants $c_{11}, c_{12}, c_{21}, c_{22}$ such that

$$U^F = c_{11}U^B + c_{12}V^B \quad (4.15)$$

$$V^F = c_{21}U^B + c_{22}V^B \quad (4.16)$$

for every x . Define

$$\Delta = u^B(v^B)' - (u^B)'v^B, \quad (4.17)$$

then after some calculation it follows that

$$c_{11} = (u^F(v^B)' - (u^F)'v^B) / \Delta \quad (4.18)$$

$$c_{12} = (u^B(u^F)' - (u^B)'u^F) / \Delta \quad (4.19)$$

$$c_{21} = ((v^B)'v^F - v^B(v^F)') / \Delta \quad (4.20)$$

$$c_{22} = (u^B(v^F)' - (u^B)'v^F) / \Delta \quad (4.21)$$

for any choice of $x \in [0, \ell]$.

From the first component of (4.15)

$$\hat{u}(\ell) = c_{11}u^B(\ell) + c_{12}v^B(\ell) = c_{11}.$$

Similarly,

$$\hat{u}'(\ell) = c_{11}u^{B'}(\ell) + c_{12}v^{B'}(\ell) = c_{12}$$

$$\hat{v}(\ell) = c_{21}u^B(\ell) + c_{22}v^B(\ell) = c_{21}$$

$$\hat{v}'(\ell) = c_{21}u^{B'}(\ell) + c_{22}v^{B'}(\ell) = c_{22}$$

Consequently, it follows from (4.2) that

$$\begin{aligned} \hat{f}(\lambda) &= \frac{\sqrt{\max\{0, 4 - [\hat{u}(\ell) + \hat{v}'(\ell)]^2\}}}{2\pi|[\hat{u}'(\ell)\sin^2\alpha + (\hat{u}(\ell) - \hat{v}'(\ell))\sin\alpha\cos\alpha - \hat{v}(\ell)\cos^2\alpha]|} \\ &= \frac{\sqrt{\max\{0, 4 - [c_{11} + c_{22}]^2\}}}{2\pi|c_{12}\sin^2\alpha + (c_{11} - c_{22})\sin\alpha\cos\alpha - c_{21}\cos^2\alpha|}. \end{aligned} \quad (4.22)$$

Since the formulas (4.18)–(4.21) are valid for any x , another approach is to recur from both ends, computing the various u_n^F, u_n^B, v_n^F , and v_n^B , or their scaled equivalents, and ‘match’ at some interior point denoted by $x = x_M$, to be determined below. In detail, we begin with

$$\tilde{u}_1^F = 1, \quad \tilde{v}_1^F = 0, \quad (\tilde{u}_1^F)' = 0, \quad (\tilde{v}_1^F)' = 1,$$

$$\tilde{u}_{N+1}^B = 1, \quad \tilde{v}_{N+1}^B = 0, \quad (\tilde{u}_{N+1}^B)' = 0, \quad (\tilde{v}_{N+1}^B)' = 1,$$

and then compute

$$\tilde{U}_{n+1}^F = A_n \tilde{U}_n^F / \sigma_n \quad (4.23)$$

$$\tilde{V}_{n+1}^F = A_n \tilde{V}_n^F / \sigma_n \quad (4.24)$$

for $n = 1, 2, \dots, M-1$, and

$$\tilde{U}_n^B = A_n^{-1} \tilde{U}_{n+1}^B / \sigma_n \quad (4.25)$$

$$\tilde{V}_n^B = A_n^{-1} \tilde{V}_{n+1}^B / \sigma_n \quad (4.26)$$

for $n = N, N-1, \dots, M$. Now from (4.13)–(4.14) and (4.17)–(4.18), with $n = M$ we have

$$\begin{aligned} c_{11} &= ((v_M^B)' u_M^F - v_M^B (u_M^F)' / (u_M^B (v_M^B)' - (u_M^B)' v_M^B)) \\ &= p(1, M-1) ((\tilde{v}_M^B)' \tilde{u}_M^F - \tilde{v}_M^B (\tilde{u}_M^F)' / [p(M, N) (\tilde{u}_M^B (\tilde{v}_M^B)' - (\tilde{u}_M^B)' \tilde{v}_M^B)]). \end{aligned}$$

Consequently, if we define the scale factor

$$\zeta_M := \frac{p(1, M-1)}{p(M, N)}, \quad (4.27)$$

then c_{11} and similarly c_{12} , c_{21} , and c_{22} given in (4.18)–(4.21) must be multiplied by ζ_M if scaled variables are used. To avoid rapid error buildup, it is desirable to have $\zeta_M \approx 1$, equivalently,

$$\begin{aligned} p(1, M-1) &\approx p(M, N) \\ &\approx \sqrt{p(1, N)} \end{aligned} \quad (4.28)$$

with M chosen to be an index for which the approximation is best. In extreme cases, products of the σ_n may overflow, so it is best to work with their logs, i.e., from (4.9), $h_n \omega_n$. Then (4.28) becomes

$$\sum_{n=1}^{M-1} ' h_n \omega_n \approx 0.5 \sum_{n=1}^N ' h_n \omega_n, \quad (4.29)$$

where the $'$ on the sum means to replace $h_n \omega_n$ with zero for any index corresponding to $\tau_n > 0$. Care must also be taken in scaling c_{11} , c_{12} , c_{21} , and c_{22} by ζ to do the quotient with the logs first and only perform the exponentiation at the end.

Hence, for a given choice of λ , the stabilized algorithm first makes an initial pass across the subintervals of $[0, \ell]$ to compute the $\{\sigma_n\}$ and M . Next, the scaled forward and backward recurrences are performed that allow the computation of c_{11} , c_{12} , c_{21} , and c_{22} . Finally (4.22) can be used to compute the estimates for $f(\lambda)$. This can be repeated for a sequence of ever finer meshes until convergence is observed. If this is not accomplished in a certain number of steps, the computation is suspended and an error flag is set.

As an illustration we choose the Mathieu equation for which

$$q(x) = \cos x. \quad (4.30)$$

We computed the spectral function $f(\lambda)$ at 101 equally spaced λ values in several stability intervals, with simple and with double shooting; the average time was measured for each method and interval. In all cases a hundred repetitions were made for each of the λ values in order for the computer clock to produce a reliable time. This was done at several tolerances on the \hat{f} sequence. The output is summarized in Table 3.1 for a Dirichlet condition at $x = 0$ corresponding to the choice $\alpha = 0$. Two absolute error tolerances were used: 10^{-6} and 10^{-8} . The ‘failure’ column shows a count of the number of values for which convergence was not achieved in eight mesh refinements (bisected uniform meshes). In Table 3.2 are the corresponding values for a Neumann condition ($\alpha = \pi/2$).

Table 4.1. Simple vs. double shooting for (4.30) – Dirichlet.

tolerance	interval	simple shooting		double shooting	
		time	# failures	time	# failures
10^{-6}	$[-0.3784, -0.3476]$	0.253	42	0.023	0
	$[0.5949, 0.9180]$	0.080	0	0.007	0
	$[1.2932, 2.2851]$	0.006	0	0.007	0
	$[2.3426, 4.0319]$	0.006	0	0.006	0
10^{-8}	$[-0.3784, -0.3476]$	0.659	96	0.042	0
	$[0.5949, 0.9180]$	0.458	51	0.013	0
	$[1.2932, 2.2851]$	0.021	0	0.021	0
	$[2.3426, 4.0319]$	0.017	0	0.017	0

Table 4.2. Simple vs. double shooting for (4.30) – Neumann.

tolerance	interval	simple shooting		double shooting	
		time	# failures	time	# failures
10^{-6}	$[-0.3784, -0.3476]$	0.300	47	0.023	0
	$[0.5949, 0.9180]$	0.110	1	0.007	0
	$[1.2932, 2.2851]$	0.007	0	0.007	0
	$[2.3426, 4.0319]$	0.009	0	0.009	0
10^{-8}	$[-0.3784, -0.3476]$	0.590	96	0.040	0
	$[0.5949, 0.9180]$	0.491	68	0.016	0
	$[1.2932, 2.2851]$	0.018	0	0.018	0
	$[2.3426, 4.0319]$	0.021	0	0.021	0

Clearly the simple shooting approach falters on the first two stability intervals. For the other two intervals the quantities τ_n in (4.4) are always positive so that theoretically the two methods should be equally reliable. The output supports this, and little time is lost from the minor overhead of the double shooting. For the remainder of the output in this paper the double shooting method always will be used.

5 Indeterminate cases

When the potential q is periodic, it is known that the spectrum exhibits spectral gaps of resolvent set where no spectrum can occur, i.e, where $f(\lambda) = 0$. Moreover, the endpoints of a spectral gap occur at values of λ^* for which $(u + v')(\ell, \lambda^*) = \pm 2$, i.e., the numerator in (3.18) vanishes. For some examples the denominator may also vanish at the same λ^* . In such cases we might expect the numerical error to be large for values of λ near such λ^* . In fact, such λ^* arise at endpoints of spectral gaps for any potential exhibiting even symmetry, i.e., $q(\ell - x) = q(x)$ for all x , as is the case for Mathieu's equation.

Case 1 (Dirichlet): assume that for some fixed $\lambda = \lambda^*$ we have $v(\ell, \lambda^*) = 0$ and $u(\ell, \lambda^*) + v_x(\ell, \lambda^*) = \pm 2$. Then, near λ^* we have

$$\begin{aligned}
4 - [u(\ell, \lambda) + v_x(\ell, \lambda)]^2 &= [2 + |u(\ell, \lambda) + v_x(\ell, \lambda)|][2 - |u(\ell, \lambda) + v_x(\ell, \lambda)|] \\
&= [2 + |u(\ell, \lambda) + v_x(\ell, \lambda)|][(u_\lambda(\ell, \lambda^*) + v_{x\lambda}(\ell, \lambda^*))(\lambda - \lambda^*) + O((\lambda - \lambda^*)^2)]
\end{aligned}$$

and

$$v(\ell, \lambda) = v_\lambda(\ell, \lambda^*)(\lambda - \lambda^*) + O((\lambda - \lambda^*)^2),$$

so that for $\lambda < \lambda^*$

$$\begin{aligned} f(\lambda) &= \frac{\sqrt{[2 + |u(\ell, \lambda) + v_x(\ell, \lambda)|]|u_\lambda(\ell, \lambda^*) + v_{x\lambda}(\ell, \lambda^*)|}}{2\pi|v_\lambda(\ell, \lambda^*)|\sqrt{\lambda^* - \lambda}} + O(\lambda^* - \lambda) \\ &\approx \frac{\sqrt{[2 + |u(\ell, \lambda) + v_x(\ell, \lambda)|]|u_\lambda(\ell, \lambda^*) + v_{x\lambda}(\ell, \lambda^*)|}}{2\pi|v_\lambda(\ell, \lambda^*)|\sqrt{\lambda^* - \lambda}}. \end{aligned} \quad (5.1)$$

Case 2: Neumann: assume that for some fixed $\lambda = \lambda^*$ we have $u_x(\ell, \lambda^*) = 0$ and $u(\ell, \lambda^*) + v_x(\ell, \lambda^*) = \pm 2$. Analogous to the Dirichlet case, we have for $\lambda > \lambda^*$

$$\begin{aligned} f(\lambda) &= \frac{\sqrt{[2 + |u(\ell, \lambda) + v_x(\ell, \lambda)|]|u_\lambda(\ell, \lambda^*) + v_{x\lambda}(\ell, \lambda^*)|}}{2\pi|u_{x\lambda}(\ell, \lambda^*)|\sqrt{\lambda - \lambda^*}} + O(\lambda - \lambda^*) \\ &\approx \frac{\sqrt{[2 + |u(\ell, \lambda) + v_x(\ell, \lambda)|]|u_\lambda(\ell, \lambda^*) + v_{x\lambda}(\ell, \lambda^*)|}}{2\pi|u_{x\lambda}(\ell, \lambda^*)|\sqrt{\lambda - \lambda^*}}. \end{aligned} \quad (5.2)$$

For a step-function potential the partial derivatives appearing in the above f formulas can be computed easily from the closed form solutions given in the previous section. The details are given in an appendix. Note that in either case we expect a $1/\sqrt{|\lambda - \lambda^*|}$ behavior near a point of indeterminacy λ^* . Our experience has shown that the expected loss of significance is not serious except (1) at very tight tolerances, (2) at values of λ very close to λ^* , or (3) near gap endpoints where the gap is very narrow (larger λ^*).

As an illustration we again choose the Mathieu potential (4.30). For an absolute error tolerance of 10^{-8} , we evaluated (3.18) and (5.1) near endpoints of the stability intervals. For (3.18) we also estimated the rate α in

$$f(\lambda) \approx \frac{\text{constant}}{|\lambda - \lambda^*|^\alpha}$$

by

$$\text{rate} \approx \frac{\log[f(\lambda_2)/f(\lambda_1)]}{\log[|\lambda_1 - \lambda^*|/|\lambda_2 - \lambda^*|]}.$$

Table 5.1 displays the numerical output for a Dirichlet initial condition, where the indeterminacy occurs at the right-hand end of a stability interval. The respective λ^* values for (5.1) are

$$\{-0.347669125306, 0.918058176625, 2.28515693444\}.$$

Table 5.2 does the same for a Neumann initial condition, where the indeterminacy is at the left-hand end of a stability interval. The λ^* values are

$$\{-0.378489221265, 0.594799970122, 1.29316628334\}.$$

Table 5.1. Behavior near an indeterminacy for (4.30) – Dirichlet.

λ	f from (3.18)	rate	f from (5.1)
-0.3497	1.34079		1.38601
-0.3493	1.50630	0.531	1.54665
-0.3489	1.74540	0.524	1.78029
-0.3485	2.13833	0.517	2.16680
-0.3481	2.98860	0.510	3.00872
-0.3477	11.23586	0.514	11.21862
0.9157	2.35819		2.35955
0.9161	2.58811	0.500	2.58938
0.9165	2.90162	0.500	2.90281
0.9169	3.36590	0.500	3.36703
0.9173	4.16048	0.500	4.16167
0.9177	6.05367	0.500	6.05564
2.2831	1.90694		1.87531
2.2835	2.11789	0.485	2.08944
2.2839	2.42382	0.488	2.39896
2.2843	2.92599	0.492	2.90536
2.2847	3.99392	0.495	3.97862
2.2851	11.27750	0.498	11.26558

Table 5.2. Behavior near an indeterminacy for (4.30) – Neumann.

λ	f from (3.18)	rate	f from (5.2)
-0.3784	5.21621	0.504	5.22961
-0.3780	2.21324	0.511	2.23105
-0.3476	1.63105	0.518	1.65468
-0.3472	1.34574	0.525	1.37416
-0.3468	1.16787	0.532	1.20046
-0.3464	1.04307		1.07943
0.5952	10.46971	0.500	10.47355
0.5956	7.40089	0.501	7.40592
0.5960	6.04084	0.501	6.04691
0.5964	5.22980	0.501	5.23678
0.5968	4.67613	0.502	4.68392
0.5972	4.26729		4.27581
1.2936	10.78605	0.500	10.77975
1.2940	7.78143	0.500	7.77625
1.2944	6.39829	0.499	6.39287
1.2948	5.56142	0.499	5.55555
1.2952	4.98576	0.499	4.97941
1.2956	4.55873		4.55190

There are slight differences between the two approaches. Since it is difficult to calculate exact answers in these cases (and λ^* itself), we have no easy way to judge which, if either, is more correct. By an inspection of intermediate quantities needed for the special formula (5.1), viz., u_λ , $v_{x,\lambda}$, they can be quite sensitive to the error in $|\lambda^* - \lambda|$, as well as the tolerance. In a more positive vein, it is clear that the double shooting method is in agreement as to the growth rate of f near λ^* in the indeterminate situations.

6 Other Numerical results

In this section we exhibit computational results illustrating the algorithms developed in the previous sections. For brevity we choose five potentials; the first is Mathieu's equation (4.30). As mentioned in the previous section, potentials such as this one that exhibit even symmetry have special properties. It can be shown that if $q(\ell - x) = q(x)$ for every x , then

$$u(\ell, \lambda) = v'(\ell, \lambda) \quad \text{for every } \lambda. \quad (6.1)$$

Moreover, whenever $|u(\ell, \lambda^*)| = 1$ for some λ^* , then either

$$v(\ell, \lambda^*) = 0 \quad (6.2)$$

or

$$u'(\ell, \lambda^*) = 0. \quad (6.3)$$

In the case (6.2), λ^* is the left endpoint of a spectral gap when y in (1.1) satisfies a Dirichlet condition. In the case of (6.3), λ^* is the right endpoint of a spectral gap when y in (1.1) satisfies a Neumann condition.

The potentials in our other examples are

$$3/(2 + \sin x), \quad (6.4)$$

$$1/\sqrt{1 - 0.75 \sin^2 x}, \quad (6.5)$$

$$(0.5 + \cos x + \cos 2x + \cos 3x)/\pi, \quad (6.6)$$

$$\sin x + 0.5 \sin 2x + 0.1 \sin 3x. \quad (6.7)$$

These have period $\ell = 2\pi$ except for (6.5) that has period π . In addition to (4.30), examples (6.5) and (6.6) also have even symmetry.

In Table 6.1a we display the endpoints of the first few stability intervals for the first two examples. For Mathieu's equation these are known [9] from the theory of elliptic cylinder functions. The numerical values agree with those found in [9], or see [4, Table I]. The numerical method used was simple binary search (bisection) seeking the zeros of

$$g(\lambda) := 2 - |u(\ell, \lambda) + v'(\ell, \lambda)|. \quad (6.8)$$

An absolute error tolerance of 10^{-8} was used in all cases. Values of f were first computed over a sufficiently fine grid to identify the locations of the gaps. As λ increases the gap width narrows, making it more difficult to isolate gap boundaries. Moreover, the loss of significance in evaluating g worsens; eventually we may have to switch to the techniques in Section 4 to help overcome this. However, this was not necessary for the data in Table 5.1a.

Table 6.1a. Stability intervals for the first two examples.

Mathieu	Example 5.4
(-0.378489, -0.347669)	(2.250000, 2.548882)
(0.594800, 0.918058)	(3.055360, 3.941647)
(1.293166, 2.285157)	(4.146186, 5.736211)
(2.342581, 4.031922)	(5.796032, 7.994726)
(4.035301, 6.270837)	(8.010349, 10.743819)
(6.270945, 9.014297)	(10.747778, 13.991464)

Similarly, Table 6.1b contains the stability intervals for Examples (6.5)–(6.7).

Table 6.1b. Stability intervals for the last three examples.

Example 5.5	Example 5.6	Example 5.7
(1.346160, 2.136962)	(0.106301, 0.247914)	(−0.419549, −0.391618)
(2.594046, 5.310602)	(0.503181, 0.995282)	(0.570873, 0.840333)
(5.452072, 10.356984)	(1.311604, 2.240365)	(1.362407, 2.217768)
(10.396276, 17.369252)	(2.602473, 4.151030)	(2.442559, 4.011052)
(17.380456, 26.372454)	(4.198967, 6.407883)	(4.078880, 6.271355)
(26.375745, 37.373218)	(6.426576, 9.160844)	(6.283327, 9.017477)

Next we compare the new formula (3.18) with a variant of the SLEDGE code. The original SLEDGE [4], [8], [10] could return estimates for the spectral measure $\rho(\lambda)$ but not for the density function $f(\lambda)$; to this code was added an implementation of interpolant 3 from [11, Eqn. (3.5)], there denoted by $(I_3\rho_b)'$, in order to provide estimates for $f(\lambda)$. Recall that SLEDGE uses the Levitan-Levinson characterization of the measure $\rho(\lambda)$. This requires the calculation of many eigenvalues and suitably normalized eigenfunctions of a regularized Sturm-Liouville problem over a finite interval $(0, b)$ for a sequence of increasingly larger b . Nevertheless, it was demonstrated in [4] that SLEDGE is capable of successfully handling a wide scope of problems. Our first example for Table 6.2a is the Mathieu equation (4.30) with a Dirichlet initial condition ($\alpha = 0$), in Table 6.2b are the data corresponding to $\alpha = \pi/6$, and in Table 6.2c are the data corresponding to a Neumann initial condition. The internal tolerance used by SLEDGE in the calculation of the eigenvalues and eigenfunctions was 10^{-6} , while for the new method it was either 10^{-6} or 10^{-8} , as shown. The final line of the table shows the computer time needed for computing f and ρ at 66 λ points. Since SLEDGE has no choice but to compute both ρ and f , we required our new method do both as well. For brevity, only some f output values and no ρ values are shown in the tables.

SLEDGE loses accuracy near the boundaries of the stability intervals, though it still seems to be converging as b increases. There is little difference in using the new formula (3.18) at the tighter tolerance, other than an increase in time. What differences there are generally occur near endpoints of stability intervals, especially when the formulas are indeterminate there. In all cases it is clear that the new approach is much faster.

Table 6.2a. Estimates of $f(\lambda)$ for Mathieu's Equation – Dirichlet.

λ	SLEDGE	SLEDGE	(3.18)	(3.18)
-0.38	0.000000	0.000000	0.00000000	0.00000000
-0.37	0.221836	0.221583	0.22149618	0.22149622
-0.36	0.439526	0.438250	0.43801179	0.43801181
-0.35	1.262850	1.247271	1.24515689	1.24515701
-0.34	0.001181	0.000591	0.00000000	0.00000000
spectral gap				
0.59	0.000029	0.000006	0.00000000	0.00000000
0.60	0.034764	0.034936	0.03503180	0.03503178
0.70	0.176067	0.175985	0.17595739	0.17595738
0.80	0.305406	0.304771	0.30451657	0.30451657
0.90	0.876650	0.855793	0.84810870	0.84810870
0.92	0.025007	0.012603	0.00000000	0.00000000
spectral gap				
1.29	0.000896	0.000195	0.00000000	0.00000000
1.30	0.028250	0.036852	0.03714803	0.03714802
1.50	0.188818	0.188736	0.18871550	0.18871550
1.75	0.268937	0.268931	0.26892936	0.26892936
2.00	0.336884	0.336798	0.33675478	0.33675478
2.25	0.673109	0.591205	0.56713172	0.56713172
2.28	0.391315	0.839088	1.23367035	1.23367034
2.30	0.267555	0.179038	0.00000000	0.00000000
spectral gap				
2.34	0.184005	0.071690	0.00000000	0.00000000
2.50	0.330775	0.330639	0.33062792	0.33062792
2.75	0.392572	0.392579	0.39258965	0.39258966
3.00	0.431331	0.431330	0.43133033	0.43133034
3.25	0.463740	0.463753	0.46375540	0.46375540
3.50	0.493118	0.493118	0.49311812	0.49311813
b	64π	128π		
tolerance	10^{-6}	10^{-6}	10^{-6}	10^{-8}
total time	72.67	246.35	0.10	0.17

Table 6.2b. Estimates of $f(\lambda)$ for Mathieu's Equation – $\alpha = \pi/6$.

λ	SLEDGE	SLEDGE	(3.18)	(3.18)
−0.38	0.000000	0.000000	0.00000000	0.00000000
−0.37	0.254422	0.254359	0.25428685	0.25428585
−0.36	0.358362	0.358111	0.35803367	0.35803367
−0.35	0.271701	0.271974	0.27213584	0.27213584
−0.34	0.000000	0.177284	0.00000000	0.00000000
spectral gap				
0.59	0.000000	0.001934	0.00000000	0.00000000
0.60	0.046178	0.046391	0.04652124	0.04652122
0.70	0.213029	0.212952	0.21292212	0.21292210
0.80	0.311584	0.311230	0.31111121	0.31111121
0.90	0.334158	0.336703	0.33591487	0.33591485
0.92	0.064154	0.065358	0.00000000	0.00000000
spectral gap				
1.29	0.018331	0.015724	0.00000000	0.00000000
1.30	0.036250	0.048914	0.04930685	0.04930685
1.50	0.225283	0.225239	0.22523166	0.22523166
1.75	0.289651	0.289648	0.28965416	0.28965416
2.00	0.327035	0.327015	0.32700588	0.32700588
2.25	0.365013	0.371550	0.36740588	0.36740588
2.28	0.550911	0.173426	0.27382995	0.27382995
2.30	1.003042	0.719051	0.00000000	0.00000000
spectral gap				
2.34	0.604674	0.435577	0.00000000	0.00000000
2.50	0.324044	0.324191	0.32423291	0.32423291
2.75	0.347326	0.347336	0.34733465	0.34733465
3.00	0.356739	0.356748	0.35675152	0.35675152
3.25	0.362111	0.362122	0.36212172	0.36212172
3.50	0.365271	0.365276	0.36527626	0.36527626
b	64π	128π		
tolerance	10^{-6}	10^{-6}	10^{-6}	10^{-8}
total time	81.45	231.55	0.09	0.14

Table 6.2c. Estimates of $f(\lambda)$ for Mathieu's Equation – Neumann.

λ	SLEDGE	SLEDGE	(3.18)	(3.18)
-0.38	0.000000	0.000000	0.00000000	0.00000000
-0.37	0.458625	0.457836	0.45743969	0.45743978
-0.36	0.231738	0.231458	0.23132070	0.23132067
-0.35	0.081480	0.081348	0.08137240	0.08137222
-0.34	0.000162	0.000080	0.00000000	0.00000000
spectral gap				
0.59	0.019597	0.009810	0.00000000	0.00000000
0.60	2.988328	2.893315	2.89226446	2.89226447
0.70	0.577118	0.576146	0.57582799	0.57582799
0.80	0.333326	0.332866	0.33272798	0.33272798
0.90	0.119832	0.119566	0.11946722	0.11946721
0.92	0.000890	0.003814	0.00000000	0.00000000
spectral gap				
1.29	0.113623	0.057586	0.00000000	0.00000000
1.30	2.917653	2.769684	2.72749873	2.72749865
1.50	0.538198	0.537216	0.53689910	0.53689910
1.75	0.376904	0.376796	0.37675762	0.37675762
2.00	0.300894	0.300884	0.30087526	0.30087526
2.25	0.162234	0.180877	0.17865547	0.17865547
2.28	0.062850	0.040850	0.08212985	0.08212987
2.30	0.160618	0.097636	0.00000000	0.00000000
spectral gap				
2.34	0.356154	0.299811	0.00000000	0.00000000
2.35	0.405038	0.440822	0.82126926	0.82126926
2.50	0.307667	0.306737	0.30645078	0.30645078
2.75	0.258179	0.258104	0.25808419	0.25808419
3.00	0.234940	0.234913	0.23490391	0.23490391
3.25	0.218489	0.218484	0.21847979	0.21847979
3.50	0.205484	0.205474	0.20547041	0.20547041
b	64π	128π		
tolerance	10^{-6}	10^{-6}	10^{-6}	10^{-8}
total time	73.64	239.55	0.09	0.16

7 Appendix: estimating variational quantities

Here we derive a method for computing the partial derivative with respect to λ of the quantities given in Section 5 for overcoming indeterminacies. Recall from Section 4 that the forward recurrence is

$$U_{n+1}^F = A_n U_n^F \quad (7.1)$$

so that

$$U_{n+1,\lambda}^F = A_{n,\lambda} U_n^F + A_n U_{n,\lambda}^F. \quad (7.2)$$

Omitting the n subscripts for now, we have

$$A_\lambda = \begin{bmatrix} \phi_{x\lambda} & \phi_\lambda \\ -\tau_\lambda \phi - \tau \phi_\lambda & \phi_{x\lambda} \end{bmatrix}.$$

But from (4.4)

$$\tau_\lambda = 1;$$

furthermore, for either sign on τ it is easily shown that at $x = x_{n+1}$

$$\phi_{x\lambda} = -h\phi/2,$$

and

$$\phi_\lambda = (h\phi_x - \phi)/(2\tau).$$

Consequently, with the n subscripts restored, a forward recursion is

$$\begin{aligned} \frac{\partial U_{n+1}^F}{\partial \lambda} &= 0.5 \begin{bmatrix} -h_n \phi_n(h_n) & (h_n \phi_{n,x}(h_n) - \phi_n(h_n))/\tau_n \\ -\phi_n(h_n) - h_n \phi_{n,x}(h_n) & -h_n \phi_n(h_n) \end{bmatrix} U_n^F \\ &+ \begin{bmatrix} \phi_{n,x}(h_n) & \phi_n(h_n) \\ -\tau_n \phi_n(h_n) & \phi_{n,x}(h_n) \end{bmatrix} \frac{\partial U_n^F}{\partial \lambda} \end{aligned} \quad (7.3)$$

with

$$\frac{\partial U_1^F}{\partial \lambda} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

The forward recurrence for $V_{n,\lambda}^F$ is identical – only the initial conditions on V_1^F differ.

A similar analysis using the A_n^{-1} as given in (4.7) leads to the backward recurrence

$$\begin{aligned} \frac{\partial U_n^B}{\partial \lambda} &= 0.5 \begin{bmatrix} -h_n \phi_n(h_n) & (\phi_n(h_n) - h_n \phi_{n,x}(h_n))/\tau_n \\ \phi_n(h_n) + h_n \phi_{n,x}(h_n) & -h_n \phi_n(h_n) \end{bmatrix} U_{n+1}^B \\ &+ \begin{bmatrix} \phi_{n,x}(h_n) & -\phi_n(h_n) \\ \tau_n \phi_n(h_n) & \phi_{n,x}(h_n) \end{bmatrix} \frac{\partial U_{n+1}^B}{\partial \lambda} \end{aligned} \quad (7.4)$$

with

$$\frac{\partial U_{N+1}^B}{\partial \lambda} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Again this holds as well for $V_{n,\lambda}^B$ with appropriate terminal values for V_{N+1}^B .

As we saw in Section 4 it is desirable to scale the variables. We will use the same notation as §4, and will first develop the formulas for \tilde{U}^F as those for \tilde{U}^B , \tilde{V}^F , and \tilde{V}^B are analogous. Following (4.13)–(4.14), we define

$$\begin{aligned} \tilde{U}_n^F &= U_n^F / p(1, n-1) \\ \tilde{U}_n^B &= U_n^B / p(n, N). \end{aligned}$$

Differentiation with respect to λ yields

$$\frac{\partial \tilde{U}_n^F}{\partial \lambda} = \frac{\partial U_n^F}{\partial \lambda} / p(1, n-1) - U_n^F \frac{\partial p(1, n-1)}{\partial \lambda} / p(1, n-1)^2.$$

But

$$\begin{aligned} -\frac{\partial p(1, n-1)}{\partial \lambda} / p(1, n-1)^2 &= [0.5/p(1, n-1)^2] \sum \frac{h_j p(1, n-1)}{\sqrt{-\tau_j}} \\ &= \sum (h_j / \sqrt{-\tau_j}) / (2p(1, n-1)), \end{aligned}$$

where the sum is taken over j , $1 \leq j < n$, for which $\tau_j < 0$. Hence,

$$\frac{\partial \tilde{U}_n^F}{\partial \lambda} = \frac{1}{p(1, n-1)} \left[\frac{\partial U_n^F}{\partial \lambda} + U_n^F \sum \frac{h_j}{\sqrt{-\tau_j}} \right], \quad (7.5)$$

and similarly

$$\frac{\partial \tilde{V}_n^F}{\partial \lambda} = \frac{1}{p(1, n-1)} \left[\frac{\partial V_n^F}{\partial \lambda} + V_n^F \sum \frac{h_j}{\sqrt{-\tau_j}} \right] \quad (7.6)$$

$$\frac{\partial \tilde{U}_n^B}{\partial \lambda} = \frac{1}{p(n, N)} \left[\frac{\partial U_n^B}{\partial \lambda} + U_n^B \sum \frac{h_j}{\sqrt{-\tau_j}} \right] \quad (7.7)$$

$$\frac{\partial \tilde{V}_n^B}{\partial \lambda} = \frac{1}{p(n, N)} \left[\frac{\partial V_n^B}{\partial \lambda} + V_n^B \sum \frac{h_j}{\sqrt{-\tau_j}} \right]. \quad (7.8)$$

$$(7.9)$$

The sums for the F -superscripted cases run from $j = 1$ to $j = n - 1$, while those for the B -superscripted cases go from $j = n$ to $j = N$. In either case, the indices for which $\tau_j > 0$ are omitted. Recall that we expect a more stable algorithm if we recur with the scaled variables, for example, using

$$\begin{aligned} \frac{\partial \tilde{U}_{n+1}^F}{\partial \lambda} &= (0.5/\sigma_n) \begin{bmatrix} -h_n \phi_n(h_n) & (h_n \phi_{n,x}(h_n) - \phi_n(h_n))/\tau_n \\ -\phi_n(h_n) - h_n \phi_{n,x}(h_n) & -h_n \phi_n(h_n) \end{bmatrix} \tilde{U}_n^F \\ &+ (1/\sigma_n) \begin{bmatrix} \phi_{n,x}(h_n) & \phi_n(h_n) \\ -\tau_n \phi_n(h_n) & \phi_{n,x}(h_n) \end{bmatrix} \frac{\partial \tilde{U}_n^F}{\partial \lambda} \end{aligned} \quad (7.10)$$

instead of (7.3). For the forward recurrences we take $n = 1, 2, \dots, M - 1$, while for the backward recurrences $n = N, N - 1, \dots, M$.

It remains to recover the desired values

$$\begin{aligned} \begin{bmatrix} u_\lambda(\ell) \\ u_{x,\lambda}(\ell) \end{bmatrix} &= \frac{\partial U_{N+1}^F}{\partial \lambda} \\ \begin{bmatrix} v_\lambda(\ell) \\ v_{x,\lambda}(\ell) \end{bmatrix} &= \frac{\partial V_{N+1}^F}{\partial \lambda} \end{aligned}$$

from the scaled variables.

From the first component of (4.15) we have for any $x \in [0, \ell]$

$$\begin{aligned} u_\lambda &= c_{11}u_\lambda^B + c_{12}v_\lambda^B + u^B \frac{\partial c_{11}}{\partial \lambda} + v^B \frac{\partial c_{12}}{\partial \lambda} \\ &= \frac{\partial c_{11}}{\partial \lambda} \quad \text{at } x = \ell. \end{aligned}$$

Similarly

$$\begin{aligned} u_{x\lambda} &= c_{11}u_{x\lambda}^B + c_{12}v_{x\lambda}^B + u_x^B \frac{\partial c_{11}}{\partial \lambda} + v_x^B \frac{\partial c_{12}}{\partial \lambda} \\ &= \frac{\partial c_{12}}{\partial \lambda} \quad \text{at } x = \ell, \end{aligned}$$

$$\begin{aligned} v_\lambda &= c_{21}u_\lambda^B + c_{22}v_\lambda^B + u^B \frac{\partial c_{21}}{\partial \lambda} + v^B \frac{\partial c_{22}}{\partial \lambda} \\ &= \frac{\partial c_{21}}{\partial \lambda} \quad \text{at } x = \ell, \end{aligned}$$

and

$$\begin{aligned} v_{x\lambda} &= c_{21}u_{x\lambda}^B + c_{22}v_{x\lambda}^B + u_x^B \frac{\partial c_{21}}{\partial \lambda} + v_x^B \frac{\partial c_{22}}{\partial \lambda} \\ &= \frac{\partial c_{22}}{\partial \lambda} \quad \text{at } x = \ell. \end{aligned}$$

Finally

$$\frac{\partial c_{11}}{\partial \lambda} = -(u_x^B u^F - v^B u_x^F) \frac{\partial \Delta}{\partial \lambda} / \Delta^2 + [v_{x,\lambda}^B u^F + v_x^B u_\lambda^F - v_\lambda^B u_x^F - v^B u_{x,\lambda}^F] / \Delta$$

and

$$\frac{\partial \Delta}{\partial \lambda} = u_\lambda^B v_x^B + u^B v_{x\lambda}^B - u_{x\lambda}^B v^B - u_x^B v_\lambda^B.$$

Similarly,

$$\frac{\partial c_{12}}{\partial \lambda} = -(u^B u_x^F - u_x^B u^F) \frac{\partial \Delta}{\partial \lambda} / \Delta^2 + [u_\lambda^B u_x^F + u^B u_{x\lambda}^F - u_{x\lambda}^B u^F - u_x^B u_\lambda^F] / \Delta$$

$$\frac{\partial c_{21}}{\partial \lambda} = -(v_x^B v^F - v^B v_x^F) \frac{\partial \Delta}{\partial \lambda} / \Delta^2 + [v_{x\lambda}^B v^F + v_x^B v_\lambda^F - v_\lambda^B v_x^F - v^B v_{x\lambda}^F] / \Delta$$

and

$$\frac{\partial c_{22}}{\partial \lambda} = -(u^B v_x^F - u_x^B v^F) \frac{\partial \Delta}{\partial \lambda} / \Delta^2 + [u_\lambda^B v_x^F + u^B v_{x\lambda}^F - u_{x\lambda}^B v^F - u_x^B v_\lambda^F] / \Delta.$$

These last five are all to be evaluated at $x = x_M$. By inspecting the scale factors, it follows that, as in Section 2, we must multiply by ζ_M given by (4.27) when using the scaled variables.

After the double-shooting and matching with scaled variables, the results are to be substituted into (5.1) or (5.2). While these formulas seem complicated, for this paper they are only to be used in the neighborhood of a 0/0. The computation of λ^* itself may be done using a characterization in terms of eigenvalues (see [4]), or by searching for zeros of the numerators in the expressions for f , (3.18), i.e., zeros of $2 - |u^F(\ell, \lambda) + v^{F'}(\ell, \lambda)| = 2 - |c_{11} + c_{22}|$.

Since we have no test problems with closed form solutions to verify computer output for the variational variables, we have compared our algorithm with finite difference approximations. Table 7.1 contains data for several of our examples with a Dirichlet initial condition. In all cases a central difference was used with a stepsize of 10^{-4} , and an absolute error tolerance of 10^{-8} was used for $u_{x\lambda}$ and v_λ . The agreement is good in all cases.

Table 7.1. Finite difference estimates compared to $u_{x\lambda}$ and v_λ .

Example	λ	$\Delta_\lambda u_x$	$u_{x\lambda}$	$\Delta_\lambda v$	v_λ
(4.30)	-0.35	-63.7915	-63.7916	-56.2402	-56.24019
	1.00	-1.6844	-1.684311	-5.2775	5.277455
	2.00	1.3092	1.309169	-2.2702	-2.270148
(6.5)	2.00	-1.7131	-1.713098	2.3125	2.312439
	3.00	0.9515	0.9514705	0.0938	0.009380
	5.00	-2.6099	-2.609927	0.6906	0.690553
(6.7)	-0.40	-5.870	-5.870013	-112.35	-112.3457
	1.00	2.6079	-2.607899	5.5210	5.521029
	2.00	1.9781	1.978065	-1.8360	-1.836113

We conclude this section with numerical data illustrating the overhead required for the additional calculation of the variational variables u_λ^F , $u_{x\lambda}^F$, v_λ^F and $v_{x\lambda}^F$. Table 7.2 has timing data for all five examples where 601 $f(\lambda)$ evaluations were made over a uniform grid of λ in the intervals shown. Examples (4.30), (6.5), and (6.7) had Dirichlet initial conditions; the other two had Neumann. The column labelled ‘basic’ gives the time required for just the u^F , u_x^F , v^F , and v_x^F calculations; the final column gives the time required to compute all eight variables.

Table 7.2. Timings for calculation of basic and variational solutions.

Example	Interval	Tolerance	Basic	All
(4.30)	[1.2, 7.2]	10^{-4}	0.027	0.031
		10^{-6}	0.048	0.086
		10^{-8}	0.103	0.120
		10^{-10}	0.126	0.149
(6.4)	[3.0, 9.0]	10^{-4}	0.036	0.041
		10^{-6}	0.078	0.121
		10^{-8}	0.146	0.164
		10^{-10}	0.180	0.203
(6.5)	[2.0, 8.0]	10^{-4}	0.040	0.046
		10^{-6}	0.090	0.117
		10^{-8}	0.162	0.178
		10^{-10}	0.198	0.222
(6.6)	[1.2, 7.2]	10^{-4}	0.048	0.054
		10^{-6}	0.143	0.162
		10^{-8}	0.196	0.214
		10^{-10}	0.368	0.524
(6.7)	[1.5, 7.5]	10^{-4}	0.050	0.056
		10^{-6}	0.138	0.169
		10^{-8}	0.204	0.224
		10^{-10}	0.336	0.510
Totals		10^{-4}	0.201	0.228
		10^{-6}	0.497	0.655
		10^{-8}	0.811	0.900
		10^{-10}	1.208	1.608

Despite the doubling in the number of dependent variables, the overhead is increased by only 10% to 30% in the totals, largely because the basic and variational variables use the same transcendental function values for a fixed λ .

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